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Evaluation of various polymers for equilibrium passive sampling of moderately hydrophobic emerging pollutants in water.

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Abstract

Passive sampling devices (PSDs) are powerful tools to measure freely dissolved contaminants (C_{free}) in water and sediment. However, PSDs have not been sufficiently developed for moderately polar contaminants, i.e. those with logarithmic octanol-water partition coefficient (log K_{ow}) ranging from 2 to 5. The goal of this study was to evaluate three polymer films for measuring C_{free} of the insecticide fipronil and its three major degradates as model compounds under equilibrium sampling conditions. Polymethylmethacrylate (PMMA) exhibited the highest affinity for fipronil and its degradates compared to polyethylene (PE) and nylon-6. Equilibrium between the target analytes and PMMA film was rapidly established (within 24 h) under laboratory conditions. Identical PMMA-water partition coefficient (K_{pw}) values were estimated by the equilibrium concentrations and from a first-order kinetics equation ($R2 > 0.83$) that was also used for PE. The average log K_{pw} of fipronil and its three degradates was 3.37 ± 0.32. In addition, we observed a tenfold increase in sorption capacity of PMMA after a 30-min swelling treatment in ethyl ether. We hypothesize that swelling modified the polymer matrix and surface structure as revealed by topography images taken by an atomic force microscope. We further applied PMMA for measurement of C_{free} for fipronil in situ in an urban waterway and also ex situ for spiked sediments.